Spin Bath Decoherence Mediated by Phonons

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Abstract

We introduce an exactly solvable model to study decoherence of a central spin interacting with a spin bath where the coupling is mediated by phonons which we assume to be in a coherent state or thermal distribution. For the coherent state case, we find that the decoherence factor decays in a Gaussian fashion and it becomes independent of the phonon frequencies at short times. If the phonon energies are much larger than spin-phonon coupling or bath spins are fully polarized, decoherence time becomes independent of the initial phonon state. For the thermal state case, phonons play more important role in decoherence with increasing temperature. We also discuss possible effects of the temperature on spin bath contribution to decoherence.

Decoherence is the key concept for understanding the emergence of classical states out of a quantum system [1]. This phenomenon is also the main challenge in quantum information processing [2]. Coupling of central two level system (qubit) to environment, leads to loss of phase relation between the states of the qubit. Therefore, the superposition of the qubit states evolves into a statistical mixture of the states, so called pointer states. These states are determined by the form of the system-environment interaction. If the qubit starts from a pure state where it is decoupled from the environment, in time, the qubit and the environment become quantum mechanically correlated. As the qubit gets entangled with the environment, it can no longer be described by a pure state. Although decoherence concept seems to solve most of the puzzle of the emergence of classicality, there are still open questions like "How does the information flow from system to environment?". Understanding this

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information transfer is believed to be crucial for explaining the objectivity of the classical world [3,4].

Being the elementary quantum information units, qubits are one of the most extensively studied open quantum systems. Especially solid state qubits (quantum dots, SQUIDs, magnetic molecules, etc.) have attracted a great interest due to their scalability which is an indispensable criterion for realistic quantum information processing. However, most important drawback of these systems is their relatively strong couplings to the environment. Understanding the mechanism of these interactions is crucial for the implementation of error correction techniques [5] and/or error avoiding strategies [6]. Starting with the pioneering works of Caldeira and Leggett [7,8], the crucial effects of environment on the dynamics of the central system has been studied with different models. Among them spin-boson model has attracted much attention [9,10]. Now, it is a well understood environmental model. However, this model is inadequate in most situations where localized environmental modes act as a main source of decoherence [11,12]. In these cases spin bath models are used to describe the environment. In spite of numerous theoretical works, including both analytical approaches [13,14,15,16,17] and numerical simulations [18,19,20,21], spin bath decoherence is still a hot subject. This is due to the rich dynamics of spin models with different intra-bath couplings. Quantum dots are extensively studied systems, both theoretically and experimentally, where the hyperfine interaction with nuclear spins is dominating mechanism of decoherence [22].

Generally, bosonic and fermionic modes are considered to be effective at different time scales and they are coupled to the qubit independently. However, this is not always the case. For instance, recent experiments on particular single molecular magnets show that these two mechanisms cooperate together [23,24]. It has been proposed that the Waller mechanism, modulation of the dipolar fields by atomic vibrations, can play an important role [25]. Phonon assisted hyperfine interaction in quantum dots is another example [26]. Deviations of the nucleus positions due to lattice vibrations modify the hyperfine coupling with electron spin. A final example can be given from optical lattices where coupling strengths between spins trapped deep inside a confining potential change with lattice oscillations. Starting with the theoretical study of Jaksch *et al.* [27], ultra-cold atomic gases in optical lattices have attracted great attention. Possibility of controlling the interactions among trapped particles is most advantageous property of these systems. This peculiarity enables to mimic various spin models such as Ising, XY, Heisenberg and so on (see for review [28]). These developments lead to various applications in quantum information processing [29] and study of spin bath decoherence in a controlled way [30,31,32].

Inspired by these observations, we introduce a pure dephasing model where the interaction of the central two-level system with environmental spins is

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mediated by phonons. Study of pure dephasing model is motivated by two observations. Firstly, dissipative processes where the energy exchange occurs between subsystems have typically longer time scales than pure dephasing processes [33]. Secondly, exact solubility of the model gives a more clear understanding of the decoherence process. We neglect the self-Hamiltonians of the central spin and the spin bath. In particular, we don't consider any interaction among the bath spins. We assume that low energy physics of the system is governed by the effective Hamiltonian

$$H = c_z \sum_{k=1}^{N} \left[\omega_{0k} + \omega_k \left(p_k^{\dagger} + p_k \right) \right] s_{kz} + \sum_{k=1}^{N} \Omega_k p_k^{\dagger} p_k \qquad (1)$$

where c_z and s_{kz} are z-components of the Pauli spin operators for central two-level system and k^{th} spin of the bath, respectively. N is the total number of environmental spins. We are using units such that the Planck and the Boltzmann constants are unity. $p_k^{\dagger}$ and p_k are the boson creation and annihilation operators with commutation relation $[p_k, p_{k'}^{\dagger}] = \delta_{k,k'}$. Energy eigenvalues of the phonon bath are Ω_k, and the coupling strengths are ω_{0k} and ω_k. Our model is similar to the one proposed by Zurek where the central two level system is directly coupled to spin bath [34]. In our model this coupling occurs with the help of oscillatory modes. When ω_k and Ω_k vanish our model reduces to Zurek's. The model Hamiltonian describes a system where the interaction between the central two-level system and the bath spins is distance dependent and this distance is modified by some vibrational modes.

First, we solve the case where the qubit is surrounded by spins almost localized at different positions, for example at lattice points of a solid. The interaction strengths between the system and a bath spins change with the distance between them. Considering the displacement of these atomic positions as macroscopic vibrations, we model them by coherent states which are the most classical states of phonons. An atom, confined in a harmonic potential, satisfies the minimum position-momentum uncertainty when it is in a coherent state which is nothing but a Gaussian wave function displaced from the origin. Furthermore, it oscillates while preserving its shape, i.e. it remains as a coherent state. We assume that initially the system and the environment are uncorrelated so that the initial wave function can be written as a product state,

$$|\Psi(0)\rangle = (c_\uparrow | \uparrow\rangle + c_\downarrow | \downarrow\rangle) \bigotimes_{k=1}^{N} (\alpha_k | \uparrow_k\rangle + \beta_k | \downarrow_k\rangle) |\lambda_k\rangle \qquad (2)$$

where $| \uparrow\rangle(| \uparrow_k\rangle)$ and $| \downarrow\rangle(| \downarrow_k\rangle)$ are normalized eigenstates of $c_z(s_{kz})$ with eigenvalues +1 and -1, respectively. Expansion coefficients satisfy $|c_\uparrow|^2 + |c_\downarrow|^2 = |\alpha_k|^2 + |\beta_k|^2 = 1$ so that $|\Psi(0)\rangle$ is normalized. $|\lambda_k\rangle$ is the coherent state corresponding to the annihilation operator p_k with eigenvalue λ_k so that $p_k|\lambda_k\rangle = \lambda_k|\lambda_k\rangle$. With the help of the harmonic displacement operators $D(\alpha) = e^{\alpha p^{\dagger} - \alpha^* p}$, Hamiltonian can be diagonalized easily. Applying the propagator e^{-itH}, we

can calculate the time evolution of the wave function which can be written as $|\Psi(t)\rangle = c_\uparrow|\uparrow\rangle|B_+(t)\rangle + c_\downarrow|\downarrow\rangle|B_-(t)\rangle$ where

$$|B_\pm(t)\rangle = \bigotimes_{k=1}^{N}\left(\alpha_k A_k^\pm|\uparrow_k\rangle|u_k^\pm\rangle + \beta_k A_k^\mp|\downarrow_k\rangle|u_k^\mp\rangle\right). \tag{3}$$

Here $|u_k^\pm\rangle$ are the coherent states with eigenvalues

$$u_k^\pm = (\lambda_k \pm \frac{\omega_k}{\Omega_k})e^{-it\Omega_k} \mp \frac{\omega_k}{\Omega_k}, \tag{4}$$

and

$$A_k^\pm = e^{i\frac{\omega_k^2}{\Omega_k}\left(t-\frac{\sin(\Omega_k t)}{\Omega_k}\right)}e^{\mp it\omega_{0k}}e^{\mp i\frac{\omega_k}{\Omega_k}(\mathrm{Re}[\lambda_k]\sin(\Omega_k t)+\mathrm{Im}[\lambda_k](1-\cos(\Omega_k t)))}. \tag{5}$$

Total density matrix is given by $\rho = |\Psi(t)\rangle\langle\Psi(t)|$. Reduced density matrix of the central system ρ_c is obtained by tracing over all the environmental degrees of freedom as $\rho_c = Tr_{bath}\rho$. In c_z-basis, the reduced density matrix is given by

$$\rho_c = \begin{pmatrix} |c_\uparrow|^2 & c_\uparrow c_\downarrow^* r \\ c_\uparrow^* c_\downarrow r^* & |c_\downarrow|^2 \end{pmatrix} \tag{6}$$

Magnitude of the off-diagonal matrix element is determined by the decoherence factor

$$r(t) = \prod_{k=1}^{N}(|\alpha_k|^2 A_k^{-*} A_k^+\langle u_k^-|u_k^+\rangle + |\beta_k|^2 A_k^{+*} A_k^-\langle u_k^+|u_k^-\rangle) \tag{7}$$

which can be written more explicitly as

$$r(t) = \prod_{k=1}^{N} e^{-4\frac{\omega_k^2}{\Omega_k^2}(1-\cos(\Omega_k t))} \left(|\alpha_k|^2 e^{-i2\omega_{0k}t-i4\frac{\omega_k}{\Omega_k}(\mathrm{Re}[\lambda_k]\sin(\Omega_k t)+\mathrm{Im}[\lambda_k](1-\cos(\Omega_k t)))}\right.$$
$$\left. +|\beta_k|^2 e^{i2\omega_{0k}t+i4\frac{\omega_k}{\Omega_k}(\mathrm{Re}[\lambda_k]\sin(\Omega_k t)+\mathrm{Im}[\lambda_k](1-\cos(\Omega_k t)))}\right). \tag{8}$$

At $t = 0$, $r = 1$ and as t increases, in general, it decays to zero which means that interference of the states $|\uparrow\rangle$ and $|\downarrow\rangle$ is totally suppressed. At short enough times we can expand the trigonometric functions by treating $\Omega_k t$'s as small parameters to obtain

$$r(t) \approx \prod_{k=1}^{N} e^{-2\omega_k^2 t^2} \left(|\alpha_k|^2 e^{-it(4\omega_k \mathrm{Re}[\lambda_k]+2\omega_{0k})} + |\beta_k|^2 e^{it(4\omega_k \mathrm{Re}[\lambda_k]+2\omega_{0k})}\right). \tag{9}$$

If either the coupling strengths ω_k's and ω_{0k}'s or coherent state eigenvalues λ_k's are random enough, the second factor in the product leads to further

suppression of the coherence factor so that r decays in Gaussian form for large N [35],

$$|r(t)| \approx e^{-t^2 \sum_k (8|\alpha_k|^2 |\beta_k|^2 (2\omega_k \text{Re}[\lambda_k] + \omega_{0k})^2 + 2\omega_k^2)}. \tag{10}$$

Therefore phonon energies do not play any role for short time decoherence of the central system. The decoherence time is determined by the coupling constants and the initial configurations of the phonons and spin bath states. It is interesting to note that even if all the bath spins are polarized in one direction, i.e. $|\alpha_k|^2 = 1$, system still loses its coherence. This behavior is a result of presence of the phonons in the environment. It is also interesting that phonon state eigenvalues (λ_k's) do not affect the decoherence time in this case. It is obvious that in the limit of $\Omega_k \to 0$ and $\omega_k \to 0$, our Hamiltonian is reduced to Zurek's model where decoherence is due to direct spin-spin interactions only without phonon contribution. In this case initial configuration of the spin bath becomes crucial.

Another interesting case is the $\Omega_k/\omega_k \to \infty$ limit where the decoherence factor $r(t) = \prod_{k=1}^N (|\alpha_k|^2 e^{-i2\omega_{0k}t} + |\beta_k|^2 e^{i2\omega_{0k}t})$. Therefore, $r(t)$ depends on the initial configuration of bath spins only and it becomes independent of the initial phonon state eigenvalues. Since the separation of energy levels of phonons becomes very high, phonon states do not change in time and remain uncorrelated to system and bath spins.

Now, we analyze the case where phonons are in a thermal equilibrium rather than a coherent state. Such a situation can physically be realized when the atoms carrying bath spins are brought in contact with a heath bath to thermalize before $t = 0$. For thermal states phonon density matrix is given by

$$\rho_p(0) = \bigotimes_k^N (1 - e^{-\frac{\Omega_k}{T}}) \sum_{n_k=0}^\infty e^{-\frac{\Omega_k n_k}{T}} |n_k\rangle\langle n_k|. \tag{11}$$

We assume that the bath spins are in a separable state at $t = 0$ as before. Since in the Hamiltonian there are no intra-bath terms for the spins, heath bath thermalizing the phonons will simply randomize the initial spin directions. As we shall discuss below, if bath spins have individual energy levels for up and down configurations, heath bath will determine the initial occupation numbers for the two possible states in accordance with the Gibbs factors. Time evolution of the total density matrix is given by $\rho(t) = e^{-iHt}\rho(0)e^{iHt}$. Using the over-completeness relation

$$1 = \frac{1}{\pi} \int d^2\lambda |\lambda\rangle\langle\lambda|, \tag{12}$$

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and the number state representation of coherent states

$$\langle n | \lambda \rangle = e^{-|\lambda|^2/2} \frac{\lambda^n}{\sqrt{n!}},$$ (13)

it is straight forward to calculate the reduced density matrix of the central system. In this case decoherence factor becomes

$$r(t) = \prod_{k=1}^{N} e^{-4\frac{\omega_k^2}{\Omega_k^2}(1-\cos(\Omega_k t))\coth(\frac{\Omega_k}{T})} (|\alpha_k|^2 e^{-i2\omega_{0k}t} + |\beta_k|^2 e^{i2\omega_{0k}t}).$$ (14)

We first note that for $\Omega_k/T \to \infty$, Eq. (14) and Eq. (8) become identical provided that $\lambda_k = 0$. This is a consistency check for two phonon states, coherent states and thermal states, that we have discussed because at low temperatures thermal state approaches the ground state of the harmonic oscillators which are nothing but the coherent states with vanishing eigenvalues.

According to Eq. (14), decoherence factor has two contributions, coming from phonons and spins. The two mechanisms act simultaneously in decoherence of the central spin. Depending upon the interaction strengths, one of them can become the dominant mechanism. At very low temperatures, where the hyperbolic cotangent term is approximately unity, the first term becomes independent of Ω_k values provided that t is small enough. For large temperatures, decoherence factor becomes an exponentially decaying function of T. It is possible to generalize the model Hamiltonian by adding a s_{kz}-dependent intra-bath term for individual spins. In this case the heath bath will not only thermalize the phonons but also it will determine the $|\alpha_k|^2/|\beta_k|^2$ ratio. For example, at very large temperatures the ratio will tend to unity and hence the spin bath will have a more important contribution to decoherence in comparison to lower temperatures.

In conclusion, we examined a spin decoherence model where the interaction with the bath spins are modified by phonons. Coherent states of phonons correspond to almost localized bath spins. In this case we find that initial decoherence rate does not depend on the phonon energies. Furthermore, for polarized bath spins it becomes independent of the initial phonon states. Thermal phonon distribution is the other case where we found an explicit solution of the model Hamiltonian. At high temperatures phonons play a more important role in the dephasing process.

Acknowledgements

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